Yang–Lee Theory for a Nonequilibrium Phase Transition

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To analyze phase transitions in a nonequilibrium system we study its grand canonical partition function as a function of complex fugacity. Real and positive roots of the partition function mark phase transitions. This behavior, first found by Yang and Lee under general conditions for equilibrium systems, can also be applied to nonequilibrium phase transitions. We consider a one-dimensional diffusion model with periodic boundary conditions. Depending on the diffusion rates, we find real and positive roots and can distinguish two regions of analyticity, which can identified with two different phases. In a region of the parameter space both of these phases coexist. The condensation point can be computed with high accuracy.

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The investigation of nonequilibrium systems is a growing field in statistical mechanics and currently attracts much attention. In this context simple models such as driven diffusive systems play a paradigmatic role similar to the Ising model in equilibrium statistical mechanics. These systems establish a simple framework in which many phenomena can extensively be studied. Moreover, driven diffusive systems can easily be mapped to other nonequilibrium models, e.g. of polymer dynamics, interface growth and traffic flow [1–4].

A hallmark of many nonequilibrium systems is the absence of detailed balance and the support of stationary states with non-vanishing currents. Hence these systems build a larger class than respective equilibrium systems and phase transitions may appear under less restrict conditions. For example, it is known that spontaneous symmetry breaking and a first-order phase transition may occur in one-dimensional nonequilibrium systems with short-range interactions [5].

In thermal equilibrium the probability measures can in principle be expressed through an appropriate ensemble. For driven systems an equally powerful concept is missing. In Ref. [6] a grand canonical partition function for nonequilibrium systems has been introduced for the first time. For the definition of this function one uses the matrix-product representation (see below) of the stationary state. Such a representation is not known for every system. But for several models it is known and, for instance, its existence is guaranteed for open reaction-diffusion models [7]. In this Letter we utilize the partition function and show that more concepts from equilibrium physics may be applied to nonequilibrium systems. We develop a Yang–Lee theory [8] giving us a very powerful method to analyze phase transitions.

We start from the grand canonical partition function $Z(x)$ and study its behavior as a function of complex fugacity x. Although only real values of the fugacity are of physical interest, the analytical behavior of thermodynamic functions can be revealed completely only by allowing the fugacity to be complex. This was first found by Yang and Lee for equilibrium systems [8]: For finite systems the roots of the grand canonical partition function $Z(x)$ are in general complex or negative if real. But in the thermodynamic limit roots may approach the positive real axis. This marks a phase transition; in equilibrium systems the pressure $p = k_{\mathrm{B}}T \lim_{V\to\infty}((1/V)\log Z)$ is non-analytical, the density $\rho = (\partial/\partial \log x)(p/k_{\mathrm{B}}T)$ is discontinuous, and one can distinguish different phases.

We show here that the above behavior of the roots of the partition function can also be found for nonequilibrium systems. By similar reasoning, one can clearly define phases and determine their properties and furthermore transfer other concepts known from equilibrium statistical mechanics to nonequilibrium systems. A new method to compute the phase transition point with great accuracy is established, as well.

To present our results let us consider an one-dimensional stochastic diffusion model with L sites and periodic boundary conditions. Each site k may be occupied by one particle of type 1 or 2, or may be vacant (denoted by 0). Starting from random initial conditions with fixed particle densities, ρ_1 and ρ_2, the particles can rearrange themselves. The only allowed processes are local interchanges conserving the number of particles: $(\alpha)_k(\beta)_{k+1} \to (\beta)_k(\alpha)_{k+1}$ with $\alpha, \beta \in \{0, 1, 2\}$. In an infinitesimal time interval $d\tau$ these diffusion processes occur with probability $g_{\alpha,\beta}\, d\tau$. Here we consider the rates:

$$g_{1,2} = q, \quad g_{2,1} = 1, \quad g_{1,0} = g_{0,2} = 1 \tag{1}$$

All other $g_{\alpha,\beta}$ are zero. The stationary state of this model has been studied recently by Monte-Carlo simulations and mean-field approximations [9]. For a snapshot of a Monte-Carlo simulation see Fig. 1. For the parameters chosen one observes one macroscopic droplet of particles which is surrounded by vacancies with a finite density of particles. This is a first sign of a first order phase transition. Increasing q the droplet shrinks and disappears for q larger than some $q_0(\rho)$; decreasing q it grows until, for $q = 1$, all particles are bound in the droplet. For $q > 1$ the position of droplet fluctuates and is fixed for

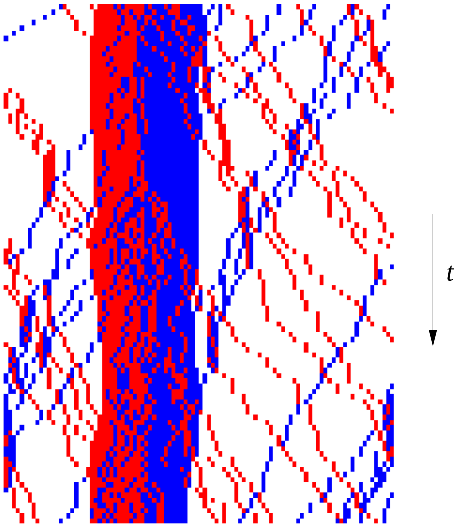

FIG. 1. A film of a Monte-Carlo simulation of the model for $q = 1.2$, $\rho_1 = \rho_2 = 0.2$ and $L = 100$. Particles of type 1 are grey and those of type 2 black.

$q < 1$, i.e. translational invariance is spontaneously broken. Similar one- and higher-dimensional models have been studied in [10,2].

The probability, $\mathcal{P}(\boldsymbol{\beta}, t)$, for configurations $\boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_L)$ at time t follows a Master Equation [1]. The stationary probability distribution $\mathcal{P}_{\rm st}(\boldsymbol{\beta})$ can be expressed as the trace over algebra elements D_β [11]:

$$\mathcal{P}_{\rm st}(\boldsymbol{\beta}) = \frac{1}{Z}\mathrm{tr}(D_{\beta_1} D_{\beta_2} \cdots D_{\beta_L}) \tag{2}$$

The normalization factor, Z, is defined as

$$Z = \sum_{\beta_1,\beta_2,\ldots,\beta_L} \mathrm{tr}(D_{\beta_1} D_{\beta_2} \cdots D_{\beta_L}) = \mathrm{tr}(C^L) \tag{3}$$

with $C = D_0 + D_1 + D_2$. In the following we recognize that Z plays the role of a grand canonical partition function. For Eq. (2) to hold, the D_β have to fulfill the quadratic algebra

$$qD_1D_2 - D_2D_1 = x_2D_1 + x_1D_2 \tag{4a}$$

$$D_1D_0 = x_1D_0 \tag{4b}$$

$$D_0D_2 = x_2D_0 \tag{4c}$$

The two free parameters x_1 and x_2 reflect the freedom to choose the two densities of particles. A representation of this algebra is known [9]

$$D_0 = \mathcal{G}_0\ , \quad D_1 = x_1\mathcal{G}_1\ , \quad D_2 = x_2\mathcal{G}_2 \tag{5}$$

with the matrices $\mathcal{G}$ given by

$$(\mathcal{G}_0)_{ij} = \delta_{1i}\delta_{1j}$$

$$\mathcal{G}_1 = \begin{pmatrix} a_1 & t_1 & 0 & 0 & \cdots \\ 0 & a_2 & t_2 & 0 & \\ 0 & 0 & a_3 & t_3 & \\ 0 & 0 & 0 & a_4 & \ddots \\ \vdots & & & & \ddots \end{pmatrix},\ \mathcal{G}_2 = \begin{pmatrix} a_1 & 0 & 0 & 0 & \cdots \\ s_1 & a_2 & 0 & 0 & \\ 0 & s_2 & a_3 & 0 & \\ 0 & 0 & s_3 & a_4 & \\ \vdots & & & \ddots & \ddots \end{pmatrix}$$

where we have introduced the notations

$$a_k = r\left(2\{k-1\}_r - \{k-2\}_r\right)$$

$$s_k\, t_k = \{k\}_r \left(3r - 1 + (2r-1)^2\,\{k-1\}_r\right)$$

$$\{k\}_r = \frac{r^k - 1}{r - 1}, \quad r = \frac{1}{q}$$

In the following we restrict ourselves to equal densities of particles, $\rho_1 = \rho_2 = \rho$, and have $x_1 = x_2 = x$. Then

$$Z = Z(x) = \sum_{\beta_1,\beta_2,\ldots,\beta_L} x^{N(\boldsymbol{\beta})}\mathrm{tr}(\mathcal{G}_{\beta_1}\mathcal{G}_{\beta_2}\cdots\mathcal{G}_{\beta_L}) \tag{6}$$

takes the form of a grand canonical partition function where $N(\boldsymbol{\beta})$ counts the number of particles in a configuration $\boldsymbol{\beta}$ and therefore x can be interpreted as a fugacity. The density of particles 1 is given by

$$\rho(x) = \frac{1}{Z}\mathrm{tr}(D_1C^{L-1}) = \frac{1}{2}\frac{\partial}{\partial \log x}P(x) \tag{7}$$

For the last expression in Eq. (7) we introduced, analogously to equilibrium physics, the "pressure"

$$P(x) = \frac{1}{L}\log Z(x) \tag{8}$$

Note, that in this context P is not the physical pressure of the particles. The singularities and the analytical behavior of $\rho(x)$ and $P(x)$ are determined by the roots of $Z(x)$. To perform a numerical calculation of $\mathrm{tr}(C^L)$ we change the ensemble slightly and require that at least one vacancy is present. In this case we have to compute $\mathrm{tr}(\mathcal{G}_0C^{L-1}) = (C^{L-1})_{11}$ which is much simpler and one has to handle $(L/2)\times(L/2)$ matrices only. Accordingly,

$$Z(x) \propto \prod_{j=1}^{L-1}(x - x_j) \tag{9}$$

is a polynomial of degree $L-1$ in x with roots x_j.

To study the analytical behavior of P and ρ we first determine the roots of $Z(x)$ in the complex plane. Since the partition function is a real polynomial with positive coefficients the roots come in complex conjugated pairs and real roots are negative. The roots of Z for two different choices $q > 1$ are shown in Fig. 2. For small q the roots are lying on an elliptic curve. For q larger than a critical value, $q_{\rm crit} \approx 2.15$, the curve is a hyperbola.

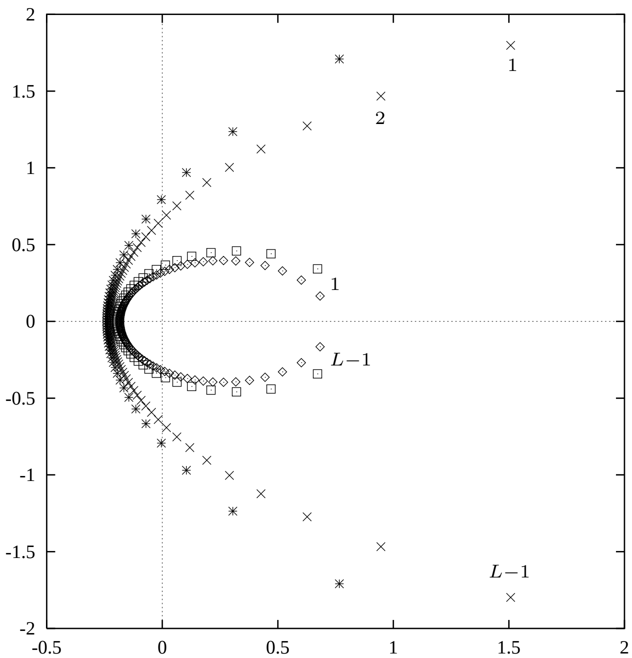

FIG. 2. The roots of Z in the complex x-plane. Shown are the $L-1$ roots for $q = 2.0$: $L = 50$ (squares) and $L = 100$ (diamonds); $q = 2.5$: $L = 50$ (stars) and $L = 100$ (crosses).

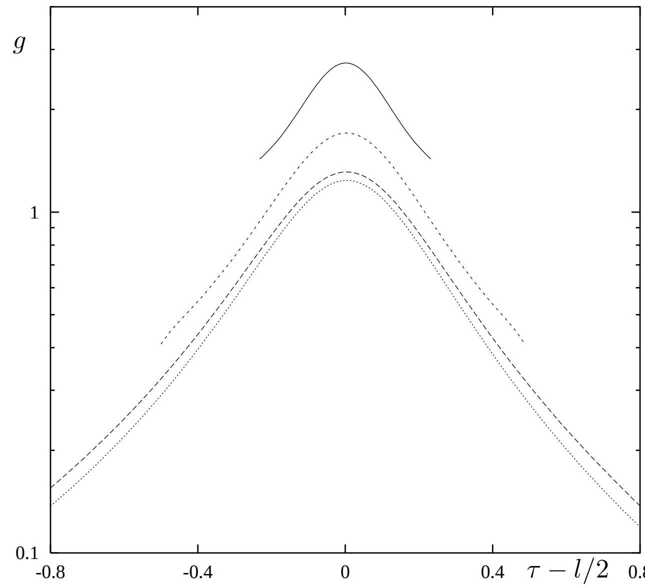

FIG. 3. The density of roots as a function of the arc length for $L = 100$ and $q = 1.2, 1.5, 2.0, 2.5$ (from top to bottom). The curve of roots in the x-plane is ellipsoidal in the first three cases and hyperbolic in the last one. The curves are shifted by half of their arclength l.

Let us treat the elliptic before the hyperbolic case. At the end we give some remarks on the case $q < 1$.

The elliptic case ($1 < q < q_{\rm crit}$). — In this case, the imaginary part of the root closest to the positive real axis (e.g. root No. 1 for $q = 2.0$ in Fig. 2) vanishes for large L with L^{-1} while the real part of this root stays finite and reaches a positive value, $\tilde{x}(q)$, in the limit $L \to \infty$.

To investigate further, let us denote the curve from the first to the last root (see Fig. 2) by $c(\tau)$ with $\tau \in [0, l]$ where l is the arclength of c. The roots are not equally spaced and their density varies with the position on the ellipse. Furthermore, with increasing system size the density of roots along the curve grows linearly in leading order and we can denote the number of roots in a line element $d\tau$ by $g(\tau)\, L\, d\tau$. The function $g(\tau)$ has a non-vanishing large L limit and is shown in Fig. 3. Since in this limit the curve $c(\tau)$ is as well defined we find the pressure (up to an additive constant)

$$P(x) = \int d\tau\, g(\tau)\, \log(x - c(\tau)) \qquad (10)$$

It is a thermodynamic quantity in the sense that its limit $L \to \infty$ exists. If $q < q_{\rm crit}$ the curve c closes to give an ellipse with a positive intercept of the real axis: $c(0) = \tilde{x} > 0$ and $g(0) > 0$ in the limit $L \to \infty$. One has to distinguish two regions of analyticity, the inner and the outer of the ellipse in the complex plane. In both regions all physical quantities are continuous and differentiable. For a plot of $P(x)$ and $\rho(x)$ see Fig. 4.

In the outer region of the ellipse ($x > \tilde{x}$) the asymptotic behavior of P is $P(x) = \log x$ and we have $\rho(x) = 1/2$ in this phase.

For x in the inner of the ellipse we find a $\tilde{\rho}$ with $\rho(x) < \tilde{\rho} < 1/2$. Crossing the ellipse at $\tilde{x}$ the pressure $P(x)$ is not differentiable and $\rho(x)$ has a finite discontinuity; the transition is of first order. The jump in the density is related to the density of roots $g(0)$ at the real axis [8]

$$1/2 - \tilde{\rho} = \pi \tilde{x} g(0) \qquad (11)$$

The value of $\tilde{x}$ can easily be obtained by extrapolating the real part of the first root for $L \to \infty$. Using Eq. (7) and extrapolating one gets $\tilde{\rho}$.

If the density ρ is fixed in the interval $\tilde{\rho} < \rho < 1/2$ one finds the two phases coexistent in the stationary state; the dense one with $\rho = 1/2$ (i.e. without vacancies) and the other with $\rho = \tilde{\rho}$ (see again Fig. 1). The dense phase acts like a bottle-neck and accordingly the current is $(q-1)\rho(1-\rho) = (q-1)/4$.

Increasing q to $q_{\rm crit}$, the density of particles above that condensation starts, $\tilde{\rho}$, reaches $1/2$ and the density of roots on the positive real axis $g(0)$ vanishes according to Eq. (11). The phases in the inner and outer region become similar and one finds a second order phase transition at $q = q_{\rm crit}$.

Next we want to fix the density of particles and determine the value $q_0(\rho)$ of q below which two phases coexist. Therefore, the values of $\tilde{\rho}$ are plotted versus q in Fig. 5. In the same plot we give the mean-field approximation for the phase transition $q_0^{\rm MF}(\rho) = (1 + 6\rho)/(1 + 2\rho)$ as it has been calculated in [9]. In the latter paper the case

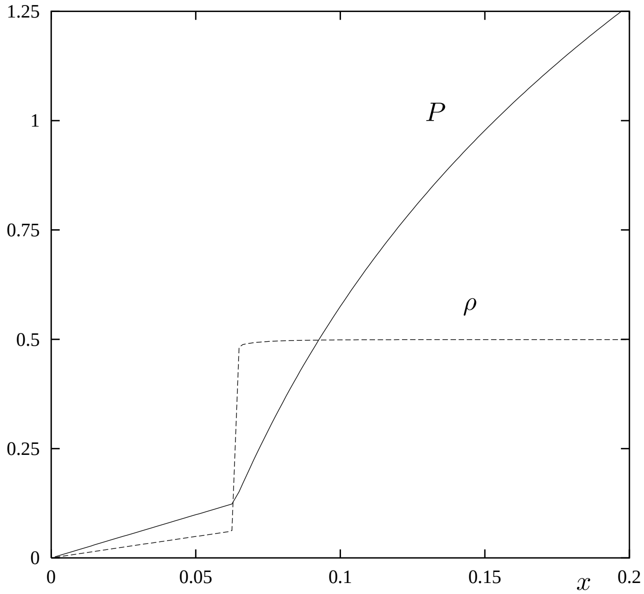

FIG. 4. The "pressure" $P = (1/L)\log Z$ and the density ρ as a function of the fugacity for $q = 1.2$ and $L = 400$.

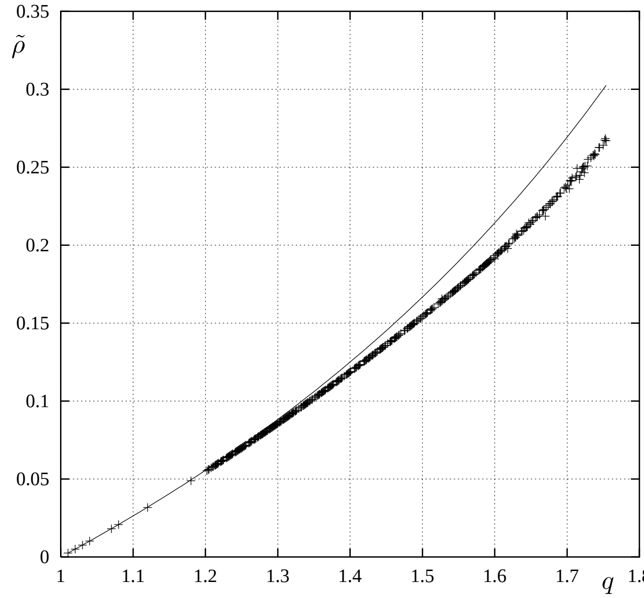

FIG. 5. The phase diagram in the ρ-q-plane. The crosses mark the phase transition obtained by the described method, the thin line results from mean-field considerations.

$\rho = 0.2$ was studied by Monte-Carlo simulations as well and the phase transition was found at $q_0^{\mathrm{MC}} = 1.62 \pm 0.05$. With the above method we find the more precise value $q_0(0.2) = 1.617 \pm 0.001$.

The hyperbolic case ($q > q_{\mathrm{crit}}$). — Also shown in Fig. 2 are the roots for $q = 2.5$. The curve $c(\tau)$ is a hyperbola. The distribution of roots $g(\tau)$ (see Fig. 3) is similar to the elliptic case. The real and imaginary part of the first and last roots, and hence the arclength, l, diverges with L. We find only the phase with $0 < \rho(x) < 1/2$ continuous and monotonically increasing with x.

The case $q < 1$. — In this case the roots lie nearly equally spaced on a circle. But the diameter of the circle shrinks exponentially with L and in the large L limit all roots are located at $x = 0$. In the limit $L \to \infty$ we find $\rho(x) = 1/2$ for $x > 0$. Details on the L-dependence and geometric properties of $c(\tau)$ for all above cases will be given elsewhere [12]. In physically interesting cases the density of particles is fixed in the interval $0 < \rho < 1/2$ and again one finds again coexistent phases.

In summary, we have demonstrated that by allowing for complex values of the fugacity in the grand canonical partition function one can analyze the phases and phase transitions in nonequilibrium models. In the model presented, a first order phase transition has been investigated. In particular, the transition point can be computed with great accuracy.

Due to the general nature of the method it can also be applied numerically or analytically to other models [12] where the density of particles controls a phase transition, e.g. jamming transitions in traffic related models. Furthermore, the method is not constrained to investigate roots in the fugacity plane. One can study complex roots of some other parameter (e.g. the input rate in the totally asymmetric exclusion process [13]) as well [12].

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